Study of α-relaxation in PVME

An Introduction to Neutron Backscattering

A. Agapov, P. Gin, E. Gomez, M. Hoarfrost, N. Osti, T.R. Prisk,
J. Wang, M. Tyagi, T. Jenkins

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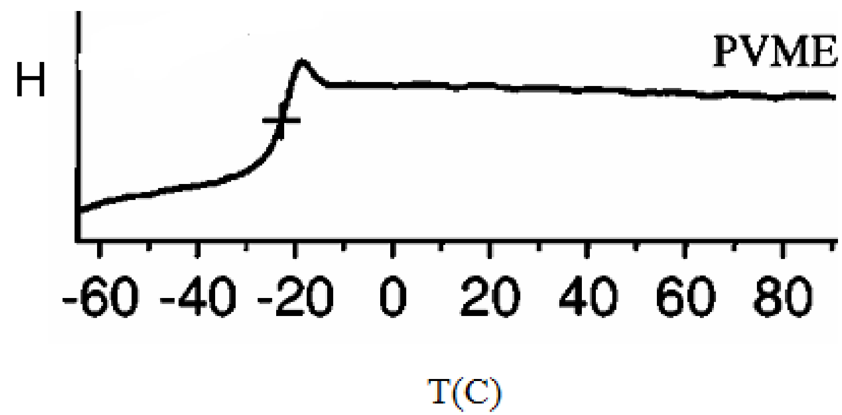
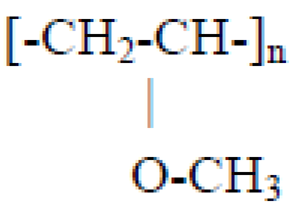
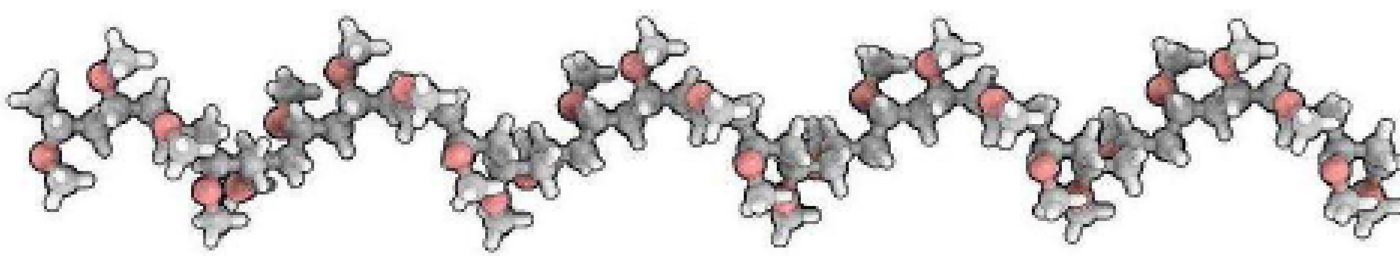
Introduction

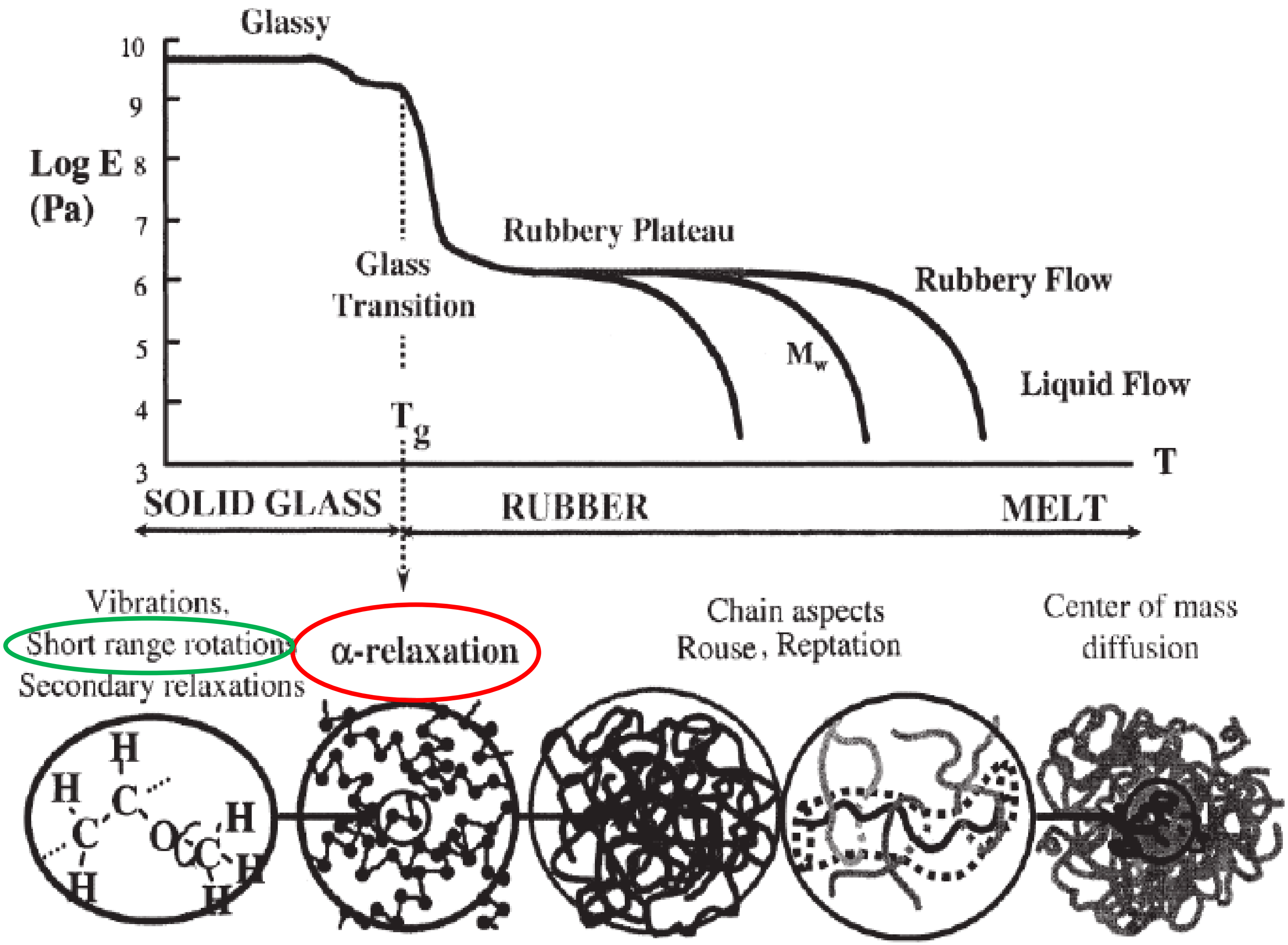
• *polymer* – molecule of high molecular mass comprised of repeating units, *monomers*, bound by covalent bonds
• useful mechanical properties as crystals, glasses, and rubbers

• **PVME** – poly(vinyl methyl ether)
• thermally agitated polymer moves at various length and time scales
•we used quasi-elastic neutron scattering (QENS) to study some of this molecular motion



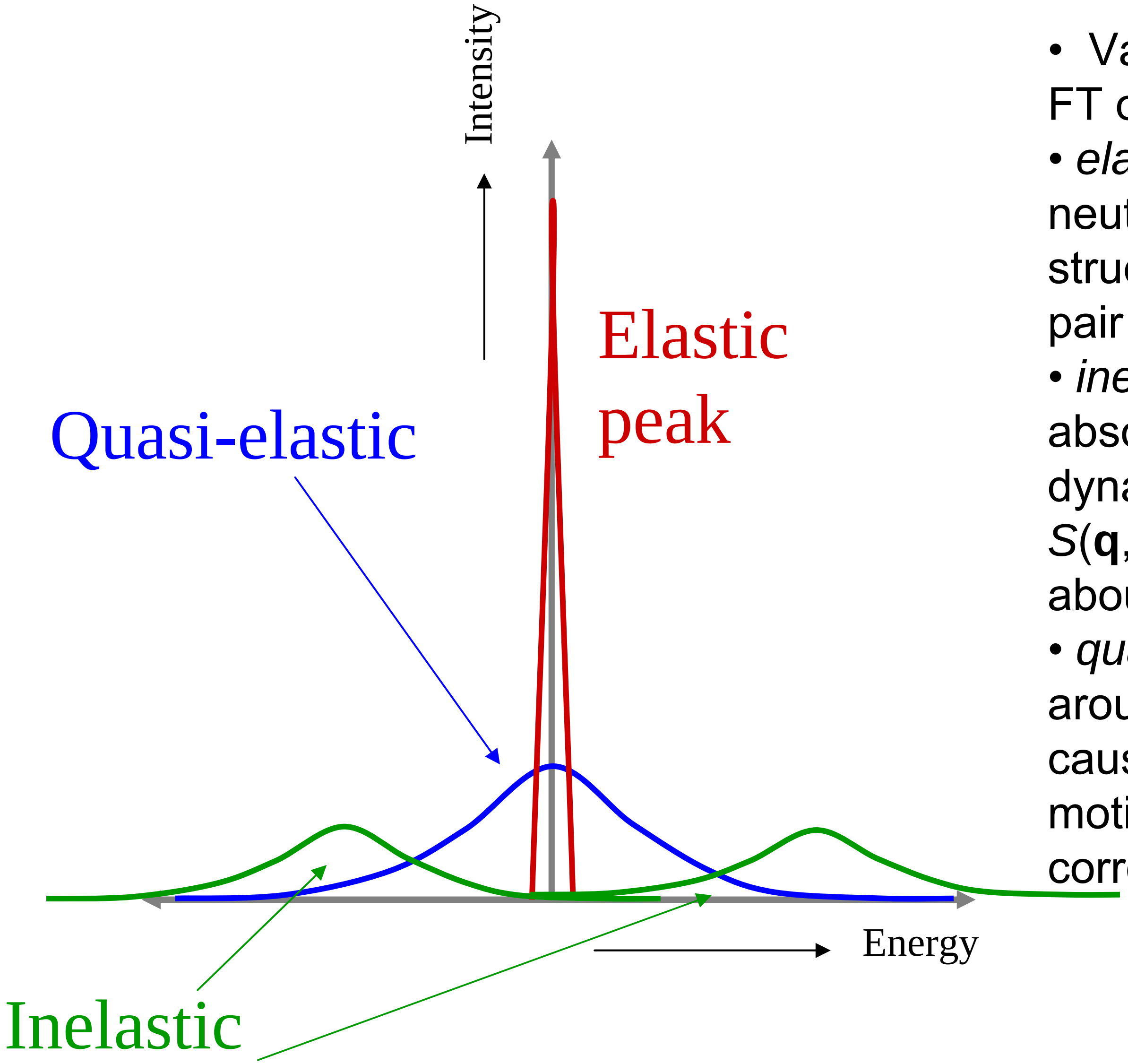




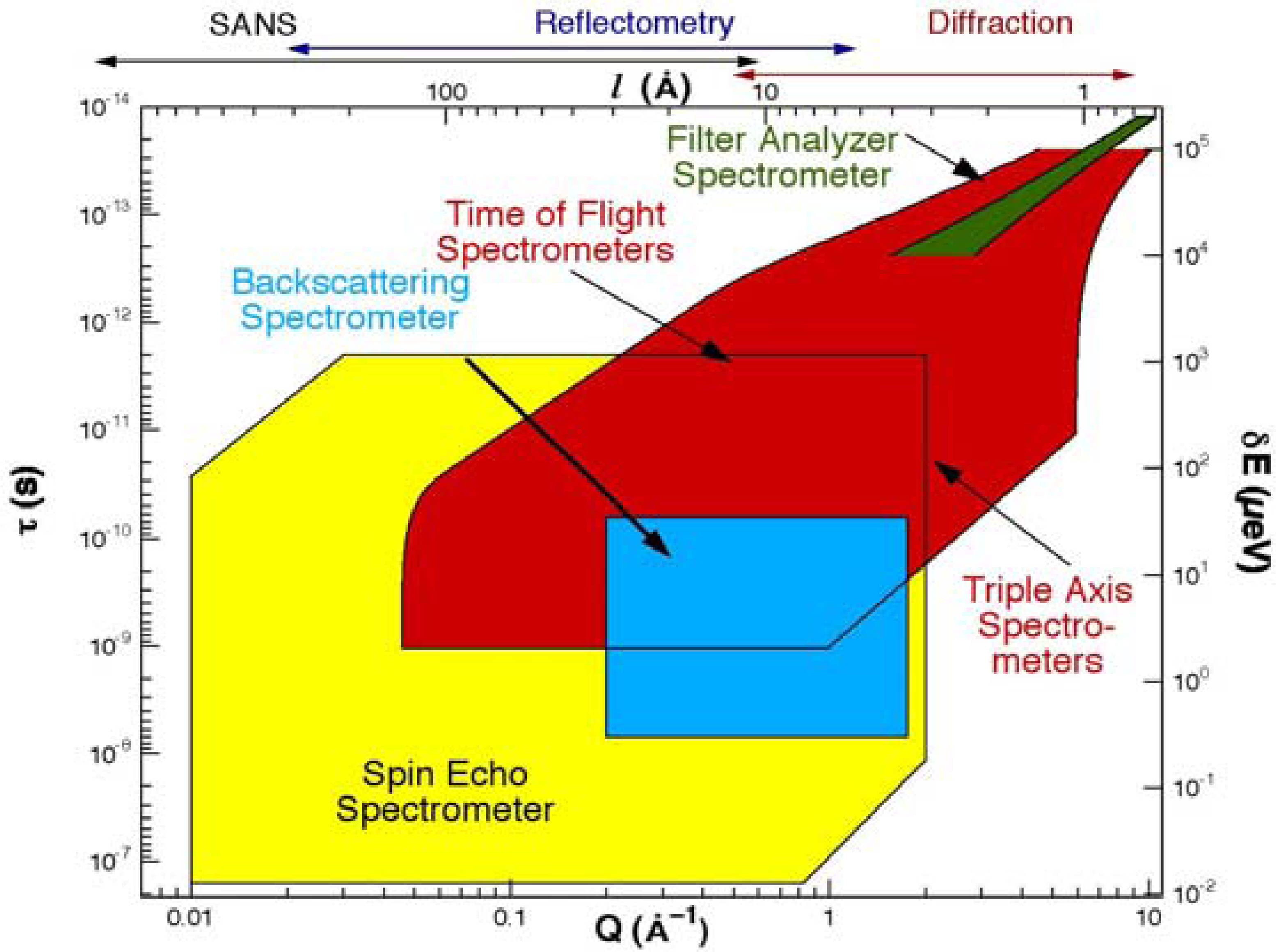


We want to characterize the monomer's diffusive motion.

What is quasi-elastic scattering?



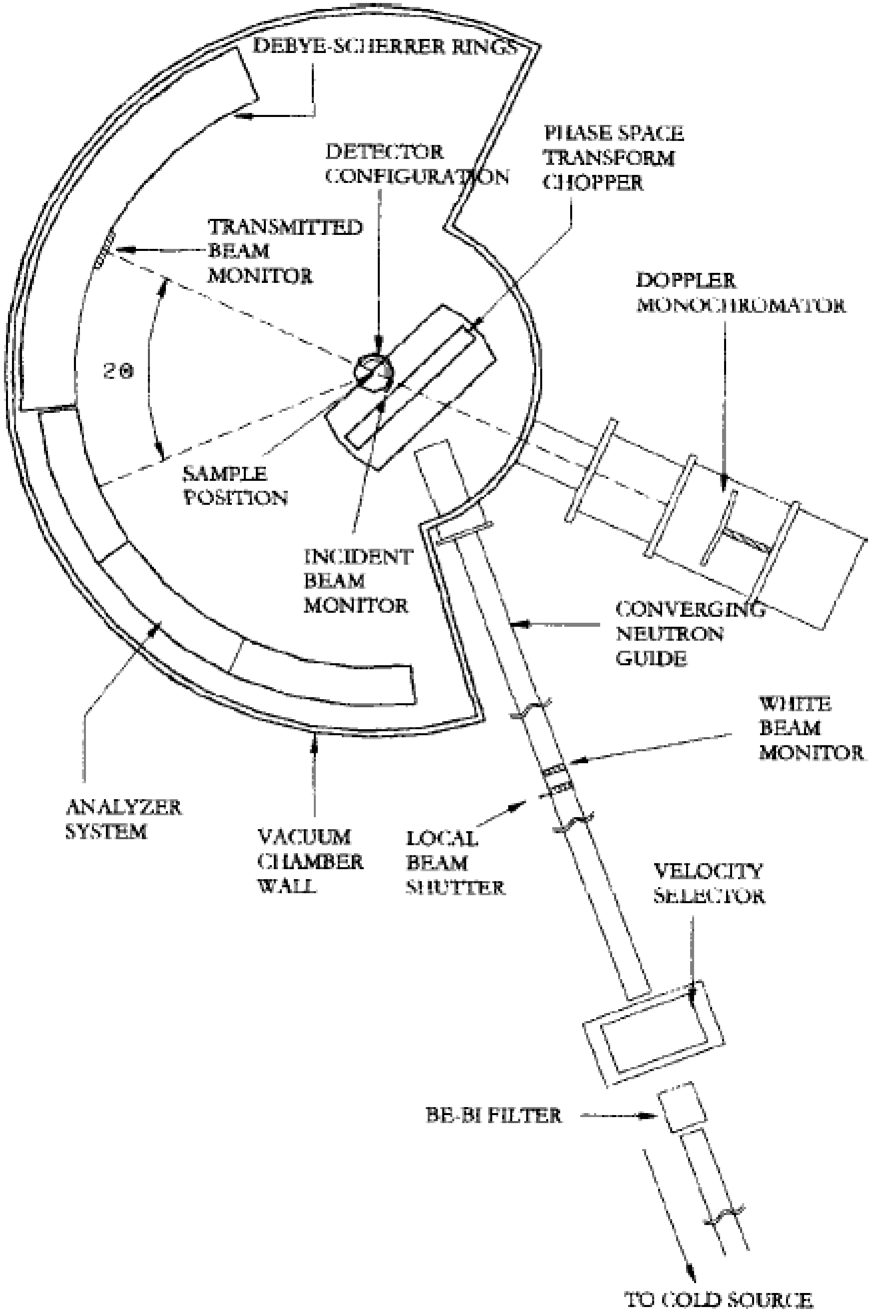
- Van Hove Law – double FT of $S(\mathbf{q},◆)$ is $G(\mathbf{r}, t)$
- *elastic* – no change in neutron energy; static structure factor $S(\mathbf{q})$ yields pair correlations
- *inelastic* – neutron emits or absorbs *n* excitations; dynamic structure factor $S(\mathbf{q},◆)$ gives information about excitations
- *quasi-elastic* – broadening around elastic peaks is caused by individual particle motion; tells you about self-correlations or diffusion



• we can probe 4-35 Å using HFBS. Monomers are typically 5 Å.

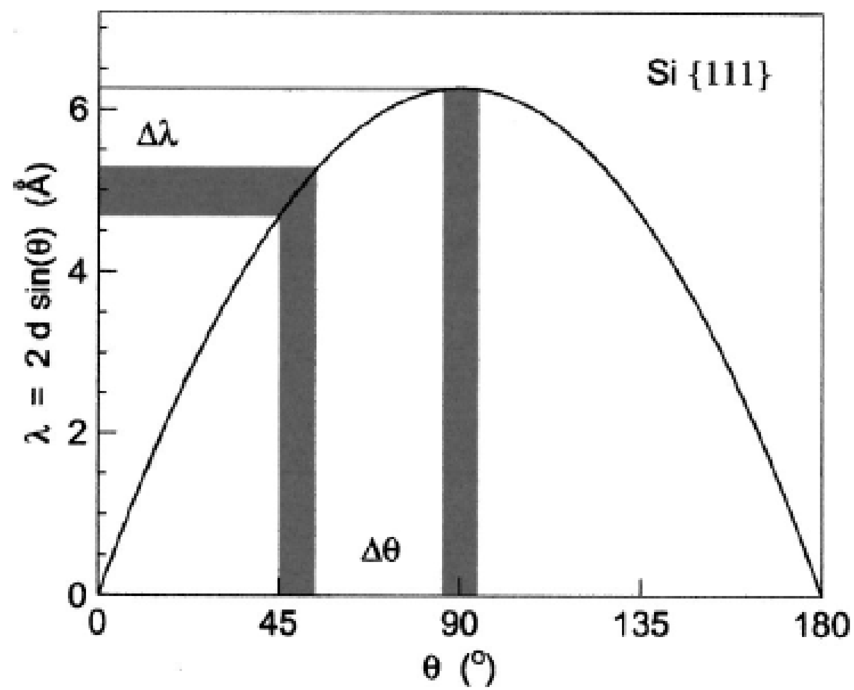
• don't need high q-resolution; would take much longer on NSE

The HFBS Instrument

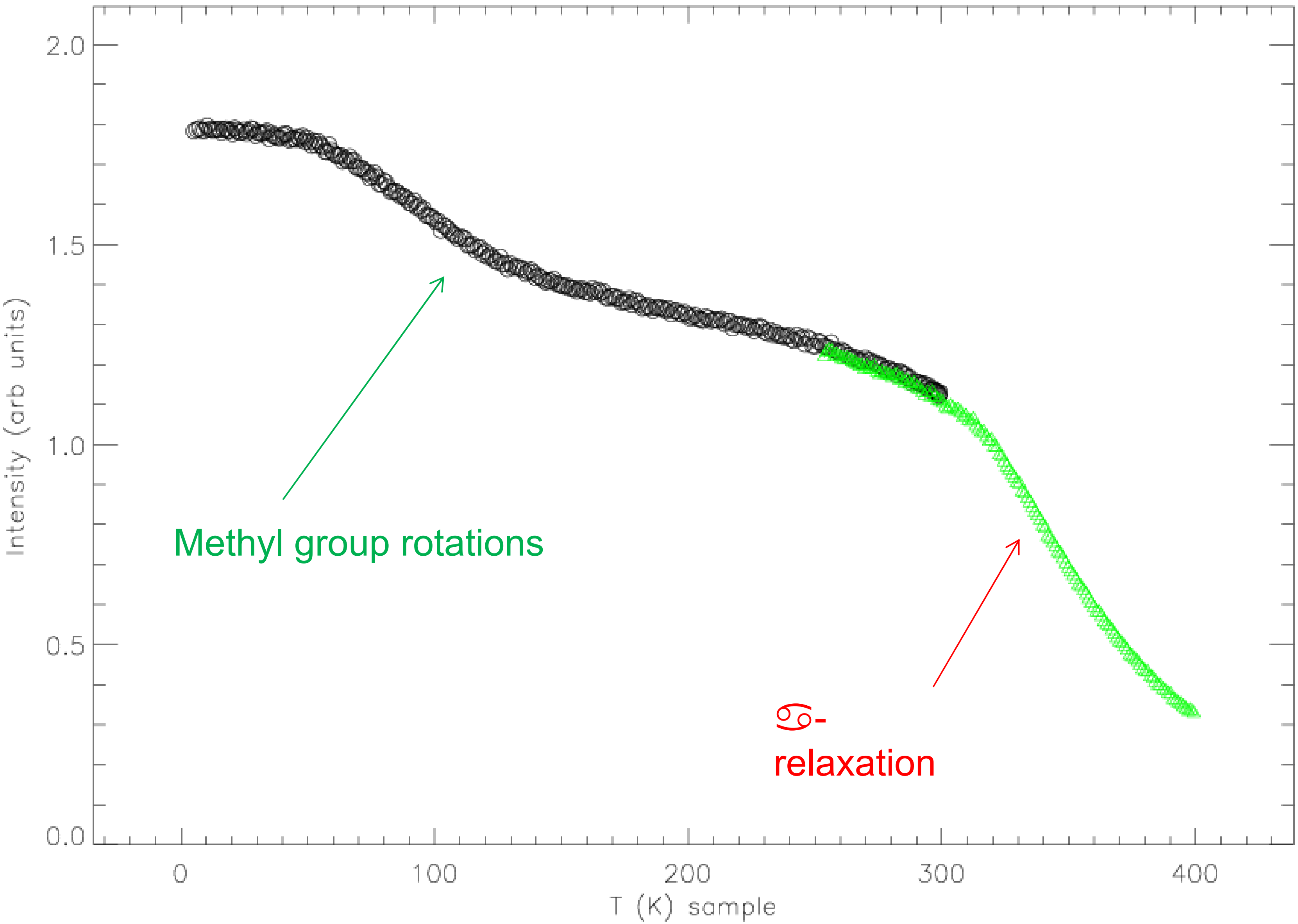


$$\frac{\delta\lambda}{\lambda} = \frac{\delta d}{d} + \frac{\delta\theta}{\tan\theta}$$

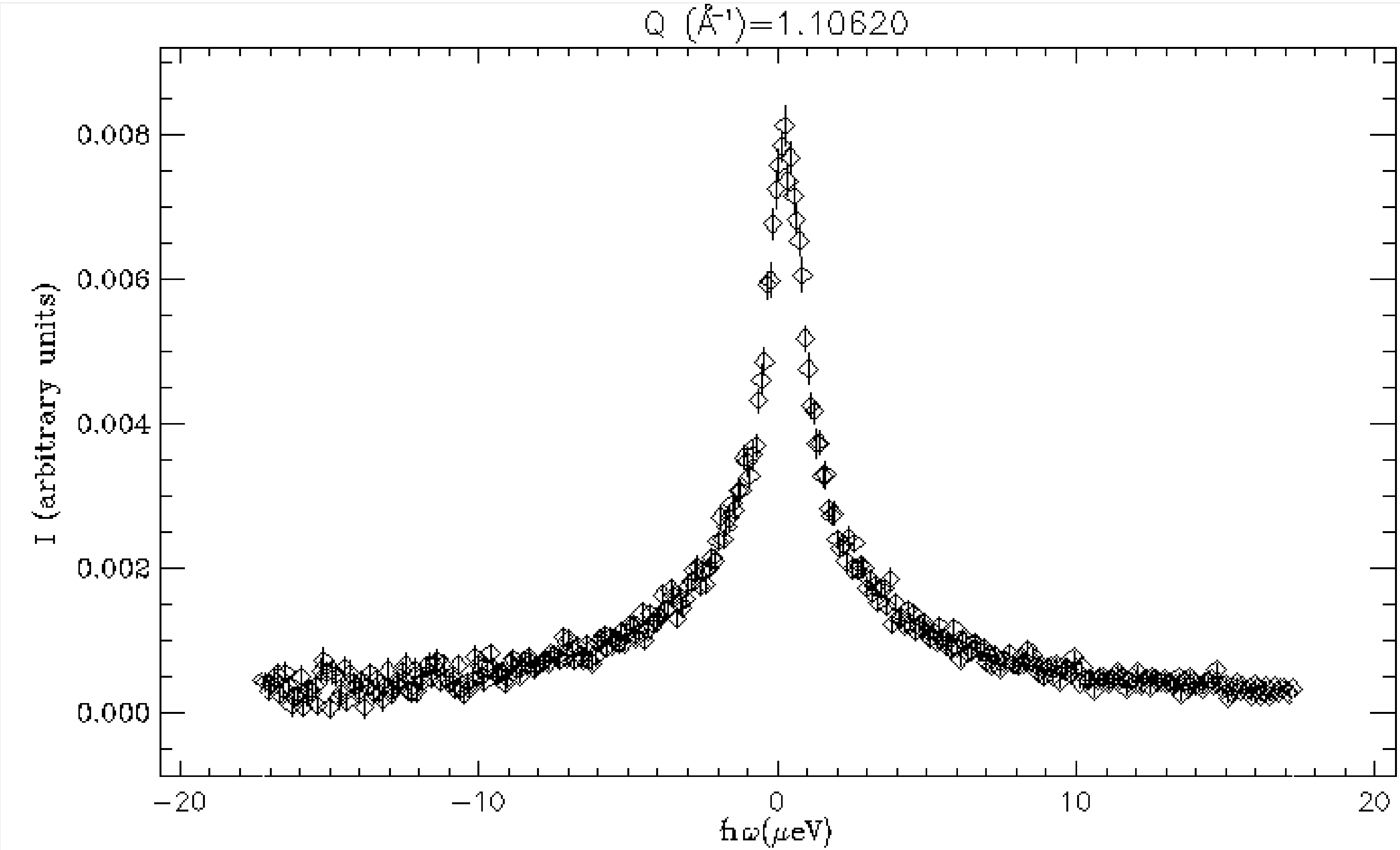
$$\approx \frac{\delta d(T)}{d(T)} + \frac{1}{8}(\delta\theta)^2$$



Fixed Window Scan



Dynamic Scan at 400 K



How to Analyze the Data

- In almost any scattering experiment, the measured data are convoluted with the resolution
- resolution in QENS determine by scattering from a standard sample with no detectable dynamics (e.g. vanadium or 4K sample)
- assume model scattering function, convolute, and then do least-squares fit
- obtain interesting dynamical factors from fit, e.g. diffusion constant *D*
- incoherent signal dominates: *self*-correlation function

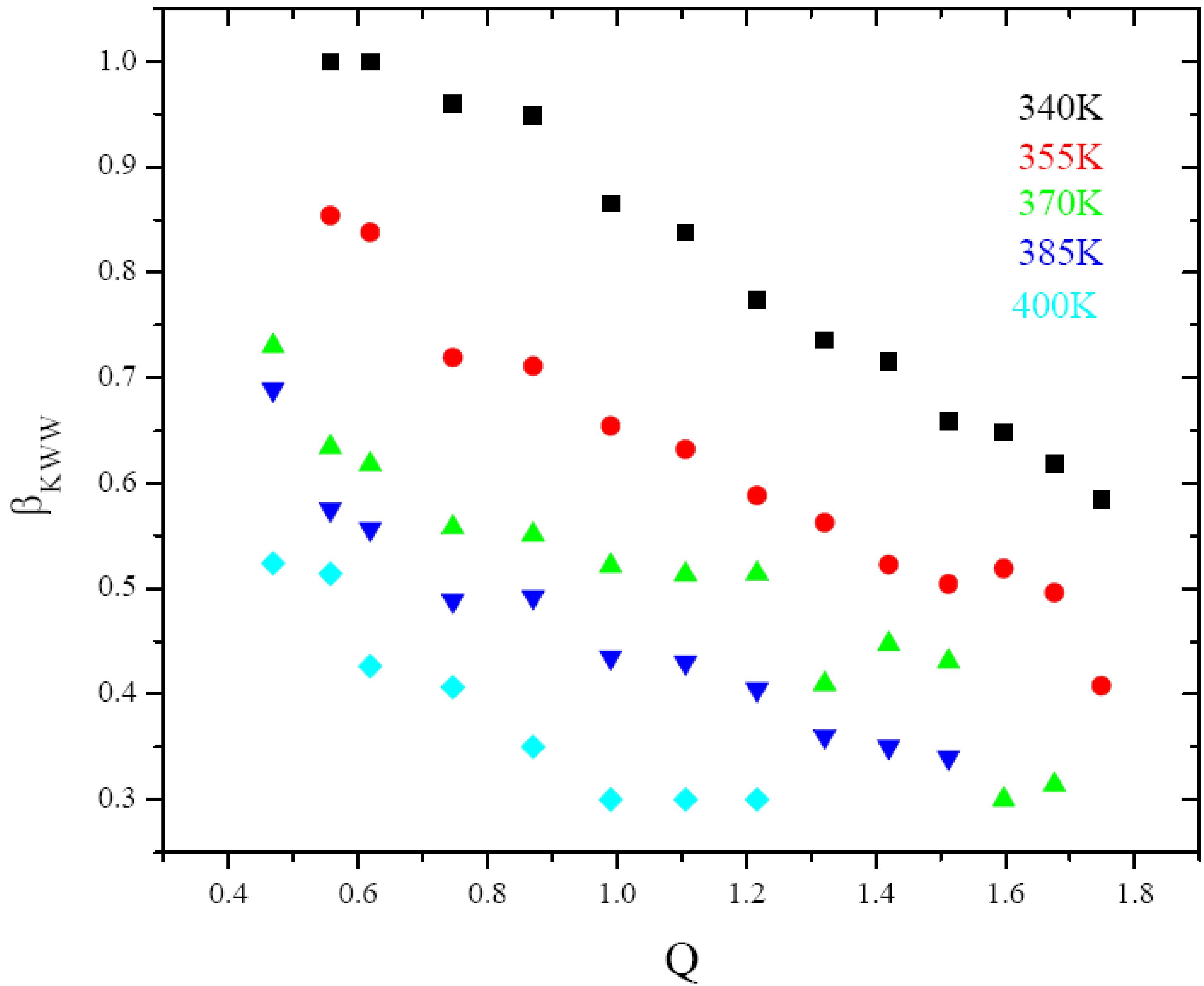
$$S_{\text{exp}}(q,\omega) = S_{\text{true}}(q,\omega) \otimes R(q,\omega)$$

$$S_{\text{brown}}(q,\omega) = \frac{1}{\pi\hbar} \frac{Dq^2}{(\hbar q^2)^2 + \omega^2}$$

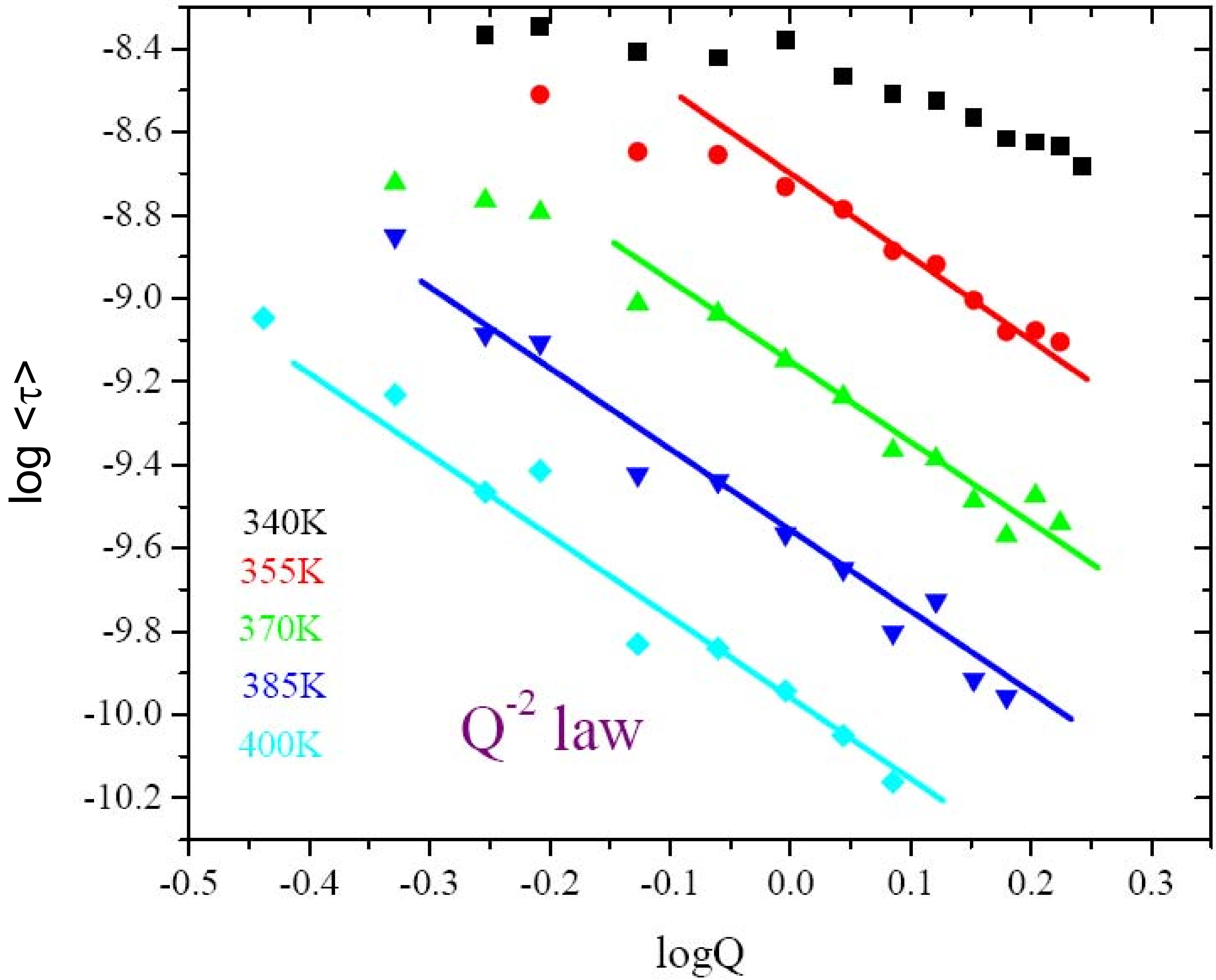
$$I(q,t) = e^{-q^2 D|t|}$$

$$S(q,t) = A(q,t) \exp[-(\frac{t}{\tau(q,T)})^{\beta(q,T)}]$$

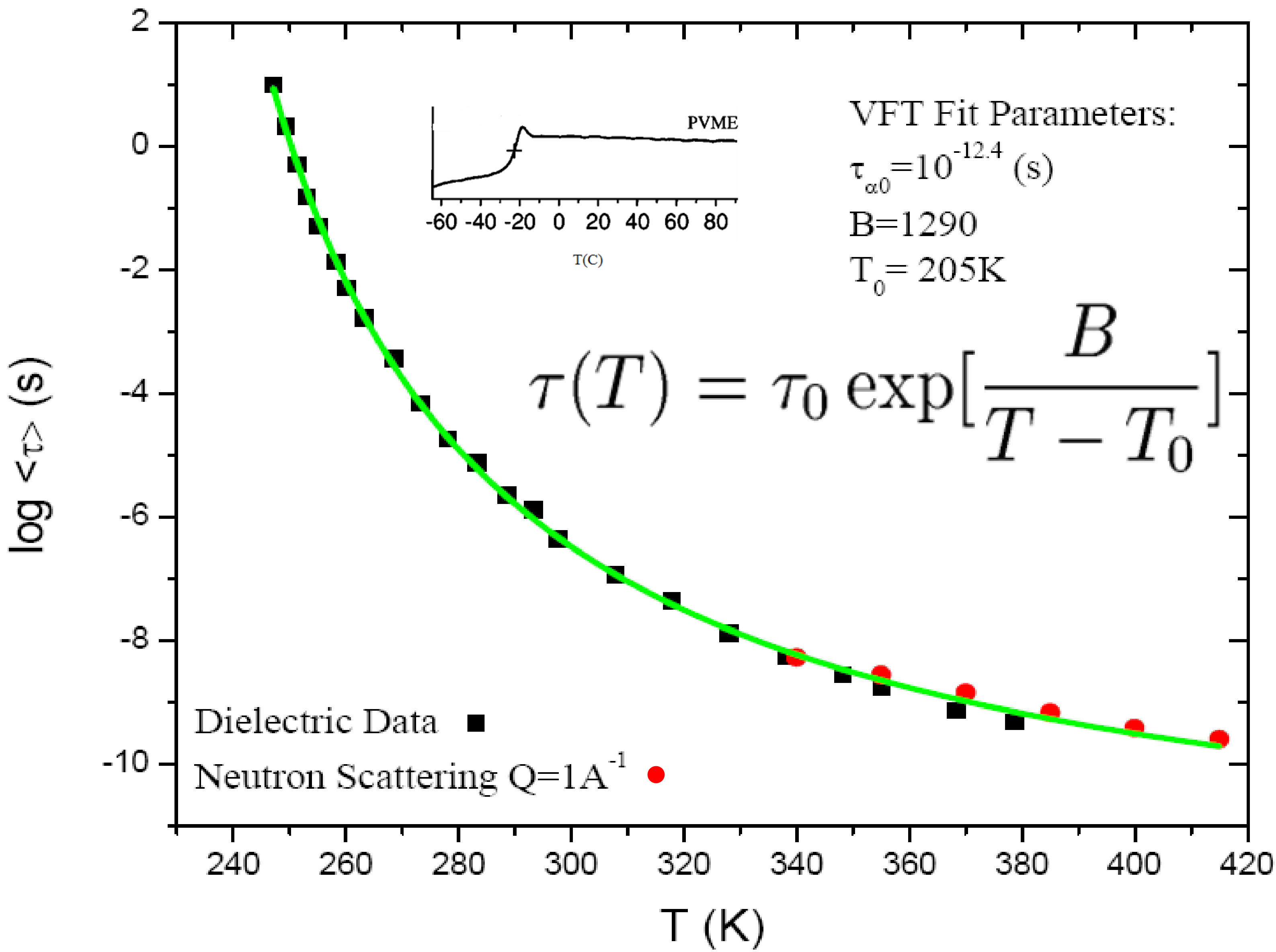
Variation with Q



Sub-diffusive motion



Vogel-Fulcher T dependence



Backscattering Rocks

- Elegant, beautiful instrument
- Well-designed
- Phase space transform chopper revolutionary
- Questions?